

Magnetocrystalline anisotropy and compositional order in $\text{Fe}_{0.5}\text{Pt}_{0.5}$: Calculations from an *ab initio* electronic model

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The magnetic properties of FePt samples, potential materials for high density recording media, depend sharply on the degree of chemical ordering produced during their preparation. This has prompted our investigation of the chemical order in both paramagnetic (*P*) and ferromagnetic (*F*) phases of a $\text{Fe}_{0.5}\text{Pt}_{0.5}$ solid solution and its effect upon the magnetocrystalline anisotropy (MAE) of the latter phase. Our “first-principles” theory uses density functional electronic structure calculations and a mean field treatment of both compositional and magnetic “local moment” fluctuations. We find both phases to be unstable to $L1_0$ (CuAu)-type order below temperatures of 1975 K (*P*) and 1565 K (*F*) which compares well with that found experimentally (≈ 1600 K) and our estimate of the Curie temperature as 575 K is also in fair agreement (710 K). For $L1_0$ order the calculated MAE is uniaxial with a simple form, $\nu_{L1_0} c_{(0,0,1)}^2 \sin^2 \theta$, where the coefficient $\nu_{L1_0} = 9.7 \times 10^8 \text{ erg/cm}^3$, $c_{(0,0,1)}$ is the degree of order (between 0 and 0.5) and θ is the angle between the magnetization direction and the magnetic easy axis, which lies perpendicular to the layering of the $L1_0$ structure, also consistent with experimental data. Tetragonal distortions of the underlying face-centered-cubic lattice that occur as chemical order sets in are found to have a much smaller effect on the MAE. © 2003 American Institute of Physics. [DOI: 10.1063/1.1523147]

I. INTRODUCTION

Alloys comprised of roughly equal proportions of iron and platinum have been investigated extensively for many years as potential permanent magnets. Below temperatures of 1600 K, a $\text{Fe}_{0.5}\text{Pt}_{0.5}$ alloy undergoes a transition from a face-centered-cubic-based solid solution into an ordered face-centered tetragonal ($L1_0$) phase,¹ which has a large value of magnetocrystalline anisotropy (MAE). Films of these alloys are easy to manufacture and are found to be chemically stable, and recent attention has been paid to high density magnetic recording² and magneto-optical recording applications.³ Since high density recording media with low noise must consist of tiny isolated grains (of size $< 10 \text{ nm}^3$), the grains need be of a high MAE material so that thermal fluctuations and demagnetizing fields, which could destabilize the magnetization of recorded bits, are avoided. Recently, nanocomposite films consisting of magnetically hard FePt nanoparticles in nonmagnetic matrices have been fabricated.^{4–7} The FePt particle composition is readily controlled, the particle diameter sizes are tuned between 3 and 10 nm, and the nanoparticles can self-assemble into 3d superlattices. Thermal annealing produces $L1_0$ order inside the particles⁸ and ferromagnetic nanocrystal assemblies can

form. These are chemically and mechanically robust and can support high density magnetization reversal transitions.

Owing to its inherent cubic symmetry, compositionally disordered $\text{Fe}_{0.5}\text{Pt}_{0.5}$ is magnetically very soft and the alloy only develops large MAE when it orders into the tetragonal $L1_0$ structure, i.e., alternately Fe then Pt layers stacked along the (1,0,0) direction. Calculations^{9–11} and measurements¹² suggest potentially the largest MAE for any purely transition metal system with a uniaxial anisotropy constant K_u of the order $\sim 10^8 \text{ erg/cm}^3$.¹³ The magneto-optical Kerr rotation also increases significantly as the degree of chemical ordering grows.^{12,13} Indeed, the magnitude of the MAE can be controlled by the extent of the ordering that is induced by annealing the films. In this article we describe results of our study of a parameter-free electronic-structure-based model of $\text{Fe}_{0.5}\text{Pt}_{0.5}$. We find the model of the solid solution to be unstable to $L1_0$ compositional ordering fluctuations below a temperature of 1975 K and the quenched disordered $\text{Fe}_{0.5}\text{Pt}_{0.5}$ alloy to be ferromagnetic below 575 K. These values are in good agreement with empirical data.¹ Crucially, from the same model, we are also able to describe the dependence of the MAE on compositional order and also to infer the structural tetragonal (c/a) distortion that accompanies ordering. The motivation for this study is to make a contribution to the modeling and tailoring of the properties of devices containing this promising magnetic material.

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The starting point is a description of the interacting electronic system in the presence of a regular lattice of sites occupied by either Fe or Pt nuclei constituting the $\text{Fe}_{0.5}\text{Pt}_{0.5}$ alloy. We use electronic density functional theory¹⁴ to accomplish this. Relativistic effects upon the electronic motions such as spin-orbit coupling are included so that MAE can be calculated.^{15–20} The effects of chemical ordering are treated by consideration of averages over the possible nuclear configurations. We model the magnetic excitations, which trigger the loss of magnetic order with rising temperature, by attaching to all lattice sites local spin-polarization axes, whose orientations vary very slowly on the time scale of the electronic motions. Appropriate ensemble averages are taken over these “local moment” degrees of freedom so that the Curie temperature and the high temperature paramagnetic phase are described. Full details of this theoretical framework can be found elsewhere,^{21–27} so only a brief overview is given here. The next section outlines the theoretical framework for compositional order in alloys pointing out how this is dependent on the magnetic state of the system. Calculations for $\text{Fe}_{0.5}\text{Pt}_{0.5}$ of the Curie temperature and chemical ordering, both above and below this transition temperature, are described next. The theory for MAE and its dependence upon compositional order is reviewed in the ensuing section together with calculations for $\text{Fe}_{0.5}\text{Pt}_{0.5}$. This section also analyzes how much of the large MAE of the ordered FePt can be assigned to the structural tetragonal distortion that accompanies ordering. Finally, a summary and conclusions are made.

II. COMPOSITIONAL ORDER

Ordering in alloys can be conveniently and succinctly classified in terms of static concentration waves.²⁸ For illustration, we consider a binary alloy A_cB_{1-c} where the atoms are arranged on a regular array of lattice sites. At high temperatures the solid solution has each of its sites occupied by either an A- or B-type atom with probabilities c and $(1-c)$, respectively. In terms of a set of site-occupation variables $\{\xi_i\}$, [with $\xi_i=1(0)$ when the i th site in the lattice is occupied by an A(B)-type atom] the thermodynamic average, $\langle \xi_i \rangle$, of the site-occupation variable is the concentration c_i at that site and for the solid solution $c_i=c$ for all sites. Below some transition temperature, T_o , the system orders or phase separates so that a compositionally modulated alloy forms. The temperature-dependent fluctuations of the concentrations about the solid solution value c , $\{\delta c_i\}=\{c_i-c\}$, can be pictured as a superposition of static concentration waves,^{21,28} i.e.,

$$c_i = c + \frac{1}{2} \sum_{\mathbf{q}} [c_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{R}_i} + c_{\mathbf{q}}^* e^{-i\mathbf{q} \cdot \mathbf{R}_i}],$$

where $c_{\mathbf{q}}$ are the amplitudes of the concentration waves with wave vectors \mathbf{q} , and \mathbf{R}_i are the lattice positions. Usually, only a few concentration waves are needed to describe a particular ordered structure. For example, (Fig. 2, top left) the CuAu-like $L1_0$ tetragonal ordered structure in an alloy with c

$=0.5$ is set up by a single concentration wave with $c_{\mathbf{q}}=\frac{1}{2}$ and $\mathbf{q}=(0,0,1)$ (\mathbf{q} is in units of $2\pi/a$, a being the lattice parameter).

Elsewhere,^{21,22,25} we have described in detail how to describe both the atomic short-range order in the compositionally disordered phase and also estimate the free energy of a partially ordered alloy in terms of a quantity $S_{ij}^{(2)}$

$$S_{jk}^{(2)}(\mathbf{e}) = - \left. \frac{\partial^2 \Omega(\{c_{ij}\}; \mathbf{e})}{\partial c_j \partial c_k} \right|_{\{c_i=c\}},$$

i.e., a second derivative with respect to concentration of the grand potential (from density functional theory) describing the interacting electron system that constitutes the alloy. $S_{ij}^{(2)}$ is formally a direct pair correlation function but can loosely be pictured as an effective atom–atom interchange energy. It is determined by the electronic structure of the disordered phase, the solid solution. The atomic short-range order, $\alpha_{ij} = \beta[\langle \xi_i \xi_j \rangle - \langle \xi_i \rangle \langle \xi_j \rangle]$, whose lattice Fourier transform $\alpha(\mathbf{q}, T)$ can be measured by diffuse scattering experiments, is related directly via $\alpha(\mathbf{q}, T) = \beta c(1-c)/[1 - \beta c(1-c)S^{(2)}(\mathbf{q})]$, where $S^{(2)}(\mathbf{q})$ is the lattice Fourier transform of $S_{ij}^{(2)}$. The spinodal transition temperature T_o , below which the alloy orders into a structure characterized by the concentration wave vector \mathbf{q}_{\max} , is determined by $S^{(2)}(\mathbf{q}_{\max})$, where \mathbf{q}_{\max} is the value at which $S^{(2)}(\mathbf{q})$ is maximal [$\mathbf{q}_{\max}=(0,0,1)$ for $L1_0$ order]. We can write,^{21,22} $T_o = c(1-c)S^{(2)}(\mathbf{q}_{\max})/k_B$. Calculations of $S^{(2)}(\mathbf{q})$ then can provide a quantitative description of the propensity of an alloy to order when thermally annealed.

As we have shown elsewhere,^{29–31} its electronic origins can determine how the state of magnetic order present at the aging temperature can affect this propensity. In the ferromagnetic state the electronic bands are spin polarized. As a metallic magnet is heated up, spin fluctuations are induced, which eventually destroy the long-range magnetic order and, hence, the overall spin polarization of the system's electronic structure. These collective electron modes interact as the temperature is raised and are dependent upon and can affect the underlying electronic structure. In many materials a simple model of local moments, which produce local magnetic fields on the lattice sites, suffices to encapsulate this behavior. The moments are assumed to vary their orientations slowly on the time scale of the electronic motions³² and to be self-consistently maintained by them. The average over the local moments' orientations produces zero overall magnetization in the paramagnetic state, but, nonetheless, the electronic structure is affected by this local moment disorder and the compositional order, which this supports can be different from that of the ferromagnetic state.³⁰

An *ab initio* implementation of this local-moment picture for finite temperature metallic magnetism, in which the electronic structure and spin fluctuations are mutually consistent, has been set up within a mean-field (MF) framework [the so-called disordered-local-moment (DLM) approach]^{23,24} and gives a fair account of the paramagnetic states of the elemental ferromagnetic transition metals and their alloys.^{27,33} For compositionally disordered $\text{Fe}_{0.5}\text{Pt}_{0.5}$ we calculate a Curie temperature of 575 K. This compares rea-

sonably well with experimental measurements of 710 K (Ref. 1) from quenched samples and shows that the energy scale of the magnetic fluctuations is captured adequately by the local moment picture. In alloys the electronic interactions, which support such thermal, local-moment, spin fluctuations at high temperatures in the paramagnetic state, are also responsible for determining the nature of compositional ordering there. Moreover, with the onset of long-range magnetic order at lower temperatures, the electronic structure takes on different features, which can provoke a different type of compositional order.

We have calculated $S^{(2)}(\mathbf{q})$ for both ferromagnetic and paramagnetic (DLM) $\text{Fe}_{0.5}\text{Pt}_{0.5}$ and our calculations provide an explanation for the experimental observation that the atomic ordering set up in $\text{Fe}_{0.5}\text{Pt}_{0.5}$ annealed at a temperature above T_c is more pronounced than that in samples aged below in the ferromagnetically ordered state. We find FePt in both paramagnetic and ferromagnetic states to be unstable to $L1_0$ -type compositional ordering modulations [$\mathbf{q}_{\text{max}} = (0,0,1)$] below temperatures of 1975 and 1575 K, respectively. These *ab initio* values also compare well with what is observed experimentally, namely, $L1_0$ -type order below temperatures of roughly 1600 K. The results show that the direct pair correlation function [atom-atom interchange], $S^{(2)}(\mathbf{q}_{\text{max}} = (0,0,1))$ is 25% greater in the paramagnetic than in the ferromagnetic state. The results suggest that samples of FePt are better aged just above the magnetic Curie temperature if significant $L1_0$ -type order is desired. This is the case if samples with strong uniaxial magnetic anisotropy are sought. We show calculations pertinent to this situation in the next section.

III. DEPENDENCE OF THE MAGNETOCRYSTALLINE ANISOTROPY OF $\text{Fe}_{0.5}\text{Pt}_{0.5}$ UPON CHEMICAL ORDER

The magnetocrystalline anisotropy of a ferromagnetic alloy with a compositional modulation can be defined in terms of the difference between the free energies of the system magnetized along two different directions annotated \mathbf{e}_1 and \mathbf{e}_2 , i.e., $\Delta F_{\text{MAE}}(\mathbf{e}_1, \mathbf{e}_2) = F(\mathbf{e}_1) - F(\mathbf{e}_2)$. If the modulation is specified by a concentration wave of amplitude c_q and wave vector \mathbf{q} , this difference can be approximately written as³⁴

$$\Delta F_{\text{MAE}}(\mathbf{e}_1, \mathbf{e}_2) \approx \Delta F_{\text{MAE}}^{\text{dis}}(\mathbf{e}_1, \mathbf{e}_2) - Y(\mathbf{q}; \mathbf{e}_1, \mathbf{e}_2) |c_q|^2, \quad (1)$$

where $Y(\mathbf{q}; \mathbf{e}_1, \mathbf{e}_2) = \frac{1}{2} [S^{(2)}(\mathbf{q}; \mathbf{e}_1) - S^{(2)}(\mathbf{q}; \mathbf{e}_2)]$, half the difference between the direct correlation function $S^{(2)}(\mathbf{q})$ for the ferromagnetic alloy magnetized along \mathbf{e}_1 and along \mathbf{e}_2 . $\Delta F_{\text{MAE}}^{\text{dis}}$ is the MAE of the completely disordered alloy.²⁶ For an alloy with atomic short-range order (ASRO) $\alpha(\mathbf{q}; T)$ the MAE is expressed

$$\Delta F_{\text{MAE}}(\mathbf{e}_1, \mathbf{e}_2) \approx \Delta F_{\text{MAE}}^{\text{dis}}(\mathbf{e}_1, \mathbf{e}_2) - \frac{1}{V_{\text{BZ}}} k_B T \int d\mathbf{q}' Y(\mathbf{q}'; \mathbf{e}_1, \mathbf{e}_2) \alpha(\mathbf{q}', T; \mathbf{e}_1). \quad (2)$$

Now $\alpha(\mathbf{q}, T; \mathbf{e}_1)$ is a structured function of \mathbf{q} with peaks located at \mathbf{q}_{max} , wave vectors of the concentration waves,

which characterize the ordered phase the alloy can form at low temperatures at equilibrium. Just above T_o , where the ASRO is pronounced, the second term becomes $\approx -c(1-c)Y(\mathbf{q}_{\text{max}}; \mathbf{e}_1, \mathbf{e}_2)$. Full details on how the dependence of MAE on compositional ordering can be calculated from *ab initio* electronic structure calculations can be found in Refs. 26 and 27. We have shown there that the numerical accuracy of the algorithms used in our calculations is to within 0.1 μeV (or 10^4 erg/cm^3). Another aspect of this approach can be obtained from calculating $S^{(2)}(\mathbf{q}; \mathbf{e})$ for different \mathbf{q} vectors, while keeping the magnetic field and magnetization direction fixed. This gives a quantitative description of the phenomenon of magnetic annealing,²⁷ in which an applied magnetic field can cause directional compositional ordering.²⁶ We have also used this approach to investigate the relation of MAE to compositional order in permalloy, $\text{Fe}_{0.5}\text{Co}_{0.5}$, $\text{Co}_{0.5}\text{Pt}_{0.5}$,³⁴ and $\text{Fe}_{0.5}\text{Pd}_{0.5}$.³⁵ We note that a nice precursor to the work here on $\text{Fe}_{0.5}\text{Pt}_{0.5}$ is given by the calculations of the MAE of $(\text{Fe}_c\text{Pt}_{1-c})_n/\text{Pt}$ superstructures.³⁶

Our calculations of the electronic structure of randomly disordered ferromagnetic $\text{Fe}_{0.5}\text{Pt}_{0.5}$ [where we assumed the experimental bulk fcc lattice spacing of 3.846 Å (Ref. 37)]²⁷ result in spin magnetic moments of 3 and 0.26 μ_B on the Fe and Pt sites, respectively, and the saturation magnetization of 1.63 μ_B/atom (1063 erg/G cm^3), close to that found experimentally.¹³ The spin-polarized electronic density of states (DOS) is almost identical to that reported previously.³⁸ As expected from its inherent cubic symmetry, our calculations of completely disordered fcc- $\text{Fe}_{0.5}\text{Pt}_{0.5}$ suggest a tiny magnetic anisotropy, $\Delta F_{\text{MAE}}[(0,0,1), (1,1,1)/\sqrt{3}] < 10 \mu\text{eV}$. To produce a large MAE in $\text{Fe}_{0.5}\text{Pt}_{0.5}$ samples, this symmetry needs to be disrupted and $L1_0$ or CuAu-type compositional ordering, both short and long ranged, does this most effectively with its structure of alternately Fe- then Pt-rich layers stacked along one of the (0, 0, 1), (0, 1, 0), and (1, 0, 0) directions. As well as the compositional modulation, there is also a tetragonal lattice distortion, which accompanies ordering of this type. It also contributes an enhancement to the MAE, which we first estimate before turning to the predominant compositional effect.

Our results are shown in Fig. 1 for the change in MAE of the completely disordered alloy as its fcc lattice is distorted into a face-centered-tetragonal one. (We have used the "frozen" atomic-sphere potential as the c/a ratio is altered,³⁴ while the cell volume is conserved.) $L1_0$ -ordered FePt is measured to have a $c/a = 0.981$,³⁷ and we find the uniaxial anisotropy constant K for the disordered alloy with this c/a , i.e., $\Delta F_{\text{MAE}} = F[\mathbf{e}_1 = (1,0,0)] - F[\mathbf{e}_2 = (0,0,1)]$, to be about 0.3 meV per atom and a magnetic easy axis along (0, 0, 1), as found experimentally. Our subsequent calculations on the enhancement of MAE by compositional order, however, demonstrate this lattice distortion to make a relatively minor contribution to the large MAE that is found in FePt alloy samples with strong compositional order.

In Fig. 2, the MAE quantities $\Delta F_{\text{MAE}}(\mathbf{e}_1, \mathbf{e}_2)$ for three compositionally modulated structures, labeled by concentration wave vectors \mathbf{q} , are presented. The values are given for complete order, i.e., where $c_q = 0.5$ in Eq. (1). The three con-

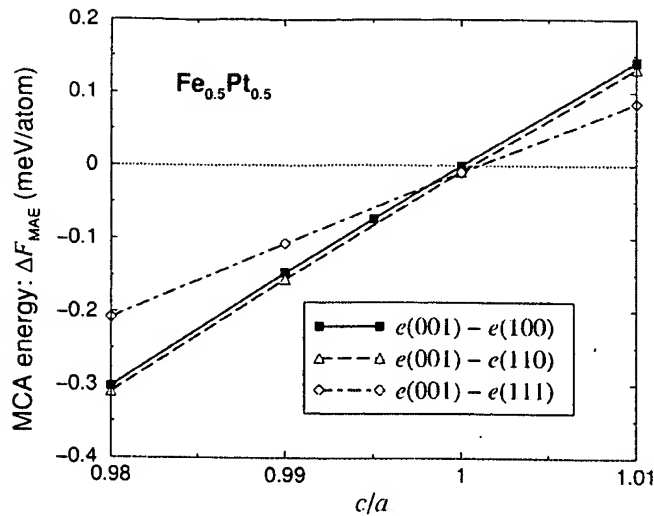


FIG. 1. Dependence of the MAE of disordered $\text{Fe}_{0.5}\text{Pt}_{0.5}$ alloy with volume-conserving fct crystal structure on c/a ratio.

figurations are shown in the upper panel of Fig. 2. It is the first structure, $L1_0$, which has the largest value and is of most practical interest. The lower panel of Fig. 2 shows the $\Delta F_{\text{MAE}}(\mathbf{e}_1, \mathbf{e}_2)$ for magnetization directions $\mathbf{e}_1 = (0,0,1)$ and $\mathbf{e}_2 = (1,0,0)$ or $(1,1,1)/\sqrt{3}$. For $L1_0$ short- or long-ranged order, the MAE is uniaxial with a simple form, $\approx \nu_{L1_0} c_{(0,0,1)}^2 \sin^2 \theta$ with $\nu_{L1_0} = 8.6 \text{ meV/atom}$ ($9.68 \times 10^8 \text{ erg/cm}^3$) and θ the angle between the magnetization and the easy axis, which is perpendicular to the layer stacking of this structure, $(0, 0, 1)$. With the amplitude of the concentration wave $c_{q=(0,0,1)}$ as 0.5, this expression yields an estimate of the uniaxial MAE constant, $K_u = \nu_{L1_0} c_{(0,0,1)}^2$, of

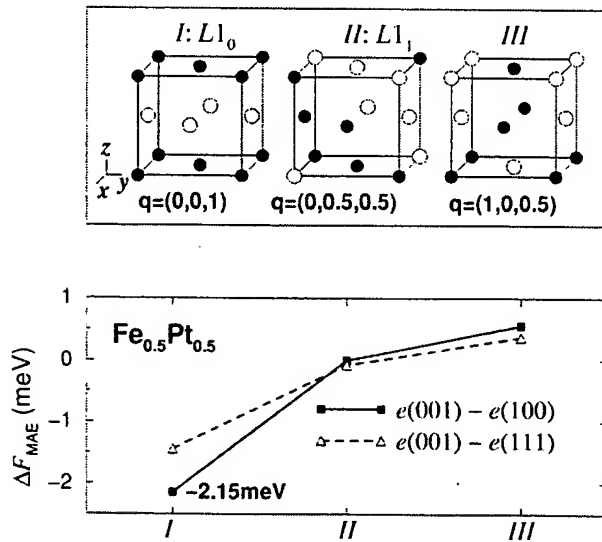


FIG. 2. Three ordered arrangements of $\text{Fe}_{0.5}\text{Pt}_{0.5}$ with their characteristic concentration wave vectors \mathbf{q} , labeled as I- $L1_0$, II- $L1_1$, and III, are shown in the upper panel. In the lower panel, the MAE energies $\Delta F_{\text{MAE}}(\mathbf{e}_1, \mathbf{e}_2)$, calculated from Eq. (1), for these ordered structures (concentration wave amplitude $c_q = 0.5$) for $\mathbf{e}_1 = (0,0,1)$ and $\mathbf{e}_2 = (1,0,0)$ and $(1,1,1)/\sqrt{3}$. When $\Delta F_{\text{MAE}} < 0$ the easy axis is along $(0,0,1)$. In the artificial configuration III, where the ordered planes of Fe and Pt are stacked along $(0,0,1)$, $\Delta F_{\text{MAE}}((0,0,1), (1,0,0)) > \Delta F_{\text{MAE}}((0,0,1), (1,1,1)/\sqrt{3}) > 0$, indicating that $(1,0,0)$ is the easy axis.

the completely ordered alloy FePt to be 2.15 meV/atom ($2.42 \times 10^8 \text{ erg/cm}^3$) and its coercivity H_c to be 210 kG. This compares well with other *ab initio* calculations that find directly the MAE of completely $L1_0$ -ordered FePt [1.75,⁹ 1.70,¹⁰ and 2.04 meV/atom]¹¹ and supports our proposal to use ν_{L1_0} and $0 < c_{(0,0,1)} < 0.5$ to estimate the MAE of samples of partially ordered FePt.

Estimates of the uniaxial MAE of ordered FePt in excess of 0.88 meV/atom (10^8 erg/cm^3) have been deduced from measurements on thin films^{12,13} at ambient temperatures. These are some of the highest values recorded for transition metal alloys. Although they are of the same order of magnitude as those calculated for completely ordered FePt, they are more than twice as small. We put this down to two main reasons: (i) the samples were likely to be incompletely ordered—our theory shows a quadratic dependence of the MAE on the order parameter $c_{q=(0,0,1)}$ [Eq. (1)], where $c_{(0,0,1)}$ can vary from 0 for the disordered alloy to 0.5 for the completely ordered one, and (ii) at ambient temperatures, thermal, local-moment fluctuations are likely to decrease MAE. We are currently developing a scheme to account for this temperature dependence in our *ab initio* calculations of MAE.

IV. CONCLUSIONS

We have investigated the chemical ordering tendencies in both the paramagnetic (P) and ferromagnetic (F) phases of a $\text{Fe}_{50}\text{Pt}_{50}$ solid solution from first principles electronic structure calculations based on electronic density functional theory. We find both phases to be unstable to $L1_0$ (CuAu) order below temperatures of 1975 K (P) and 1565 K (F), which compares well with that found experimentally (1600 K, approximately). Because effects of thermally induced local moment fluctuations are included, our electronic description of this alloy also enables us to determine the Curie temperature as 575 K, which is in reasonable agreement with the experimental value of 750 K.

Using the same electronic basis, we have investigated the magnetocrystalline anisotropy MAE with *ab initio* calculations. We find that both short- and long-ranged CuAu-type chemical order generates a significant uniaxial MAE of form $\nu_{L1_0} c_{(0,0,1)}^2 \sin^2 \theta$, where $\nu_{L1_0} = 9.7 \times 10^8 \text{ erg/cm}^3$, $c_{(0,0,1)}$ the degree of order (between 0 and 0.5), and θ is the angle between the magnetization direction and the magnetic easy axis, which lies perpendicular to the layering of the $L1_0$ structure, also consistent with experimental data. Tetragonal distortions of the underlying fcc lattice, which occur as chemical order sets in, are inferred to have a much smaller effect on the MAE. Our results show that samples annealed at temperatures above the Curie temperature will develop greater degrees of compositional order than those aged just below, and consequently such samples, when quenched, will possess larger MAE. We expect that these results may contribute to the modeling and design of devices containing this promising magnetic material.

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